GDSA Framework: Comparison of Sensitivity Analysis Methods Applied to a Reference Case Repository in Shale

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Abstract

The United States Department of Energy is developing a state of the art performance assessment simulation software toolkit, *Geologic Disposal Safety Assessment (GDSA) Framework* [Sevougian et al. 2018], that couples increasingly higher fidelity models of subsystem processes into total system performance assessment simulations, propagates uncertainty, and offers a variety of methods for sensitivity analysis. Because the total system representing a deep geologic nuclear waste repository is highly coupled and nonlinear, methods of sensitivity analysis that do not assume linearity or monotonicity and that can quantify interactions between input parameters may be desirable. We compare several methods of sensitivity analysis using a reference case nuclear waste repository in a shale formation as a test case.

Shale Reference Case

Simulations assume a mined repository for commercial nuclear waste in a thick unit of low-permeability shale. A thin limestone aquifer lies below the shale and a sandstone aquifer lies above the shale. A second sandstone aquifer lies at depth. A pressure gradient drives regional flow from west to east. Multiphysics simulations are performed with PFLOTRAN [Lichtner et al. 2018]. The model domain contains 6,925,936 cells. On 512 processes each simulation takes approximately 3 hours to run to 1 million years.

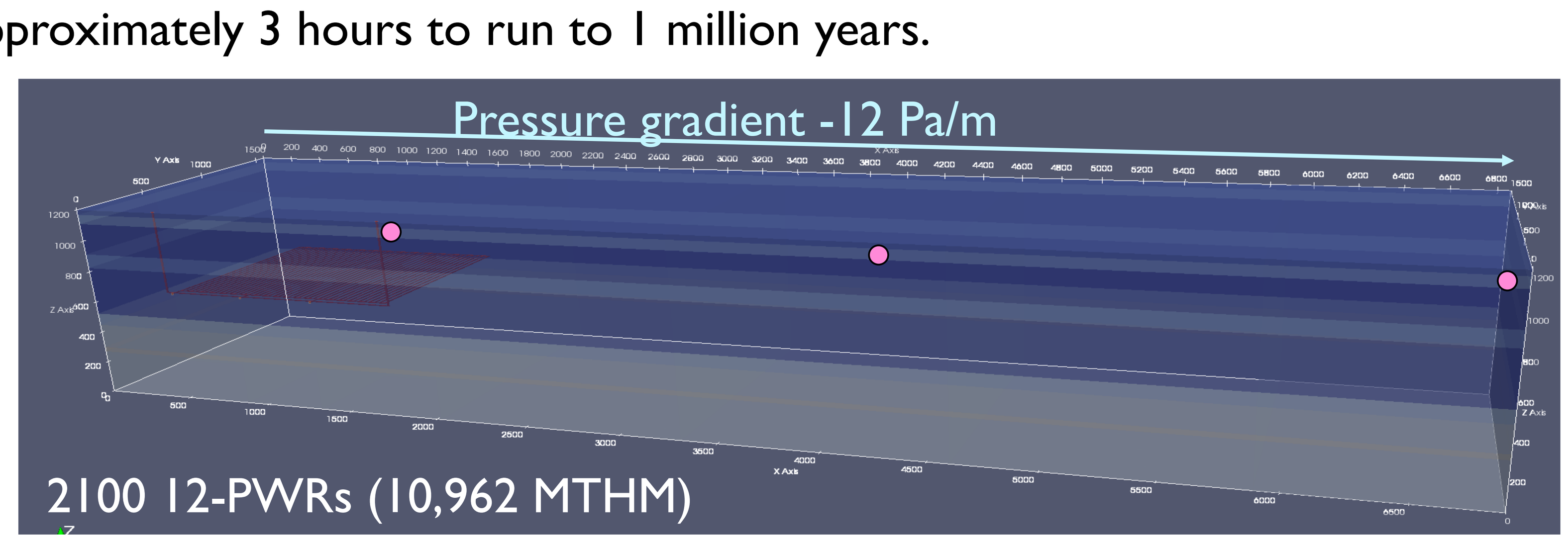

Figure 1. Model domain with locations of observation points.

Sampled Inputs

Two hundred realizations were generated using Latin Hypercube Sampling (Table 1). Concentration of ^{129}I was monitored at three observation points in the sandstone (Figure 1 and Figure 2). The maximum ^{129}I concentrations (regardless of time) at these locations are the output variables (also called response functions) for the sensitivity analysis (Figure 3). Sampling and sensitivity analyses are performed with Dakota [Adams et al. 2018].

	Description	Range	Units	Distribution
rateSNF	SNF Dissolution Rate	$10^{-8} - 10^{-6}$	yr^{-1}	log uniform
rateWP	Mean Waste Package Degradation Rate	$10^{-5.5} - 10^{-4.5}$	yr^{-1}	log uniform
kSand	Upper Sandstone k	$10^{-15} - 10^{-13}$	m^2	log uniform
kLime	Limestone k	$10^{-17} - 10^{-14}$	m^2	log uniform
kLSand	Lower Sandstone k	$10^{-14} - 10^{-12}$	m^2	log uniform
kBuffer	Buffer k	$10^{-20} - 10^{-16}$	m^2	log uniform
kDRZ	DRZ k	$10^{-18} - 10^{-16}$	m^2	log uniform
pShale	Host Rock (Shale) ϕ	0.1 – 0.25	-	uniform

Table 1. Sampled input variables.

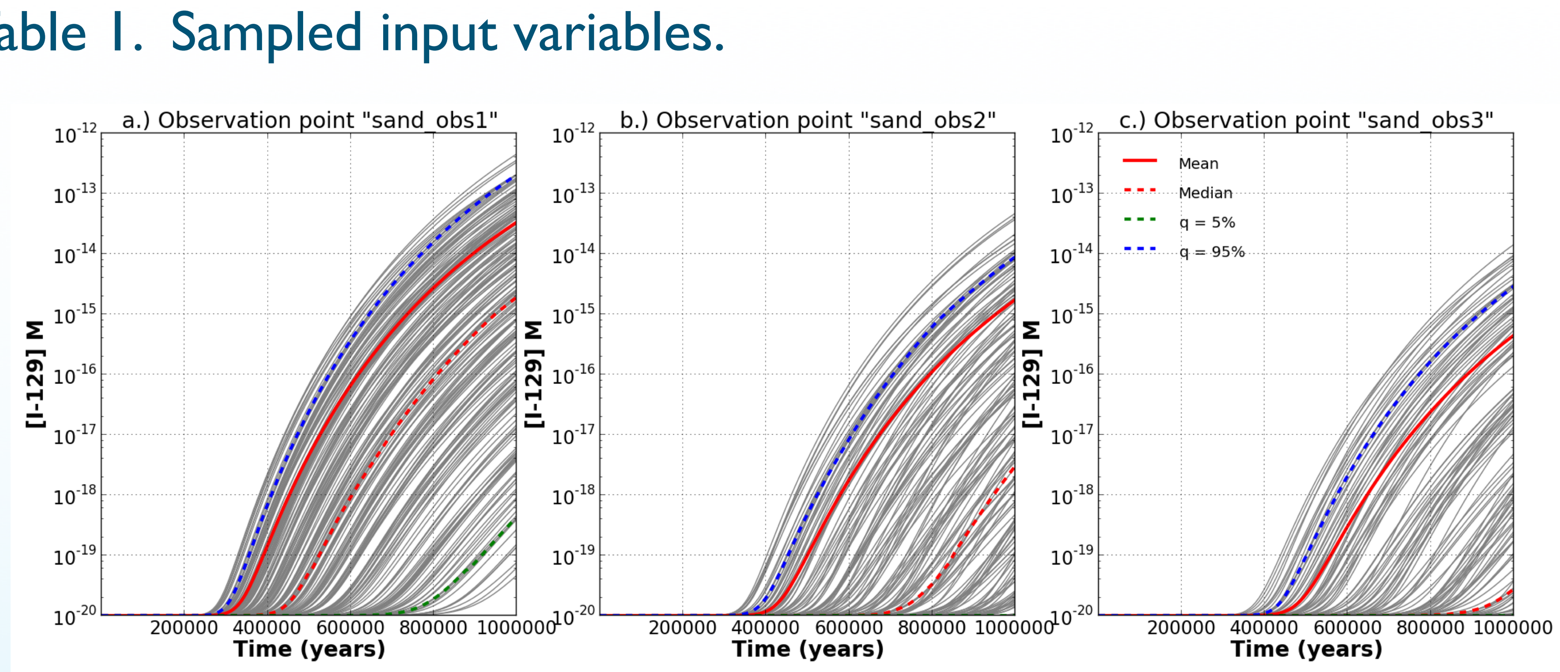

Figure 2. ^{129}I concentration v. time at the observation points.

Sensitivity

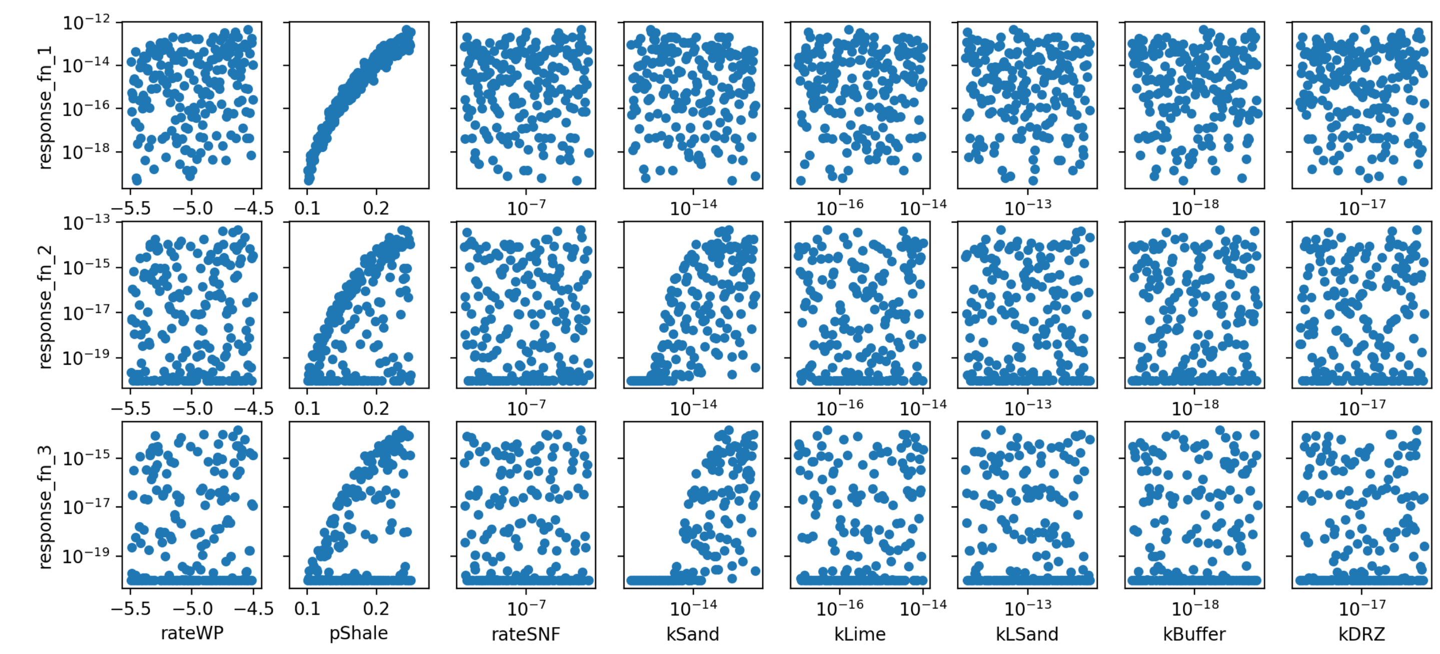

Figure 3. Maximum ^{129}I concentration as a function of sampled inputs.

- Simple and partial correlation coefficients measure linear correlation.
- Partial correlation removes the effects of other variables.
- Standardized regression coefficients are calculated from stepwise multiple linear regression.
- Ranks transformation improves correlation for monotonic but nonlinear relationships.
- Sensitivity indices equal the fraction of variance in the output due to the variance in an input. Those presented here are calculated from Gaussian process and polynomial chaos expansion surrogate models.

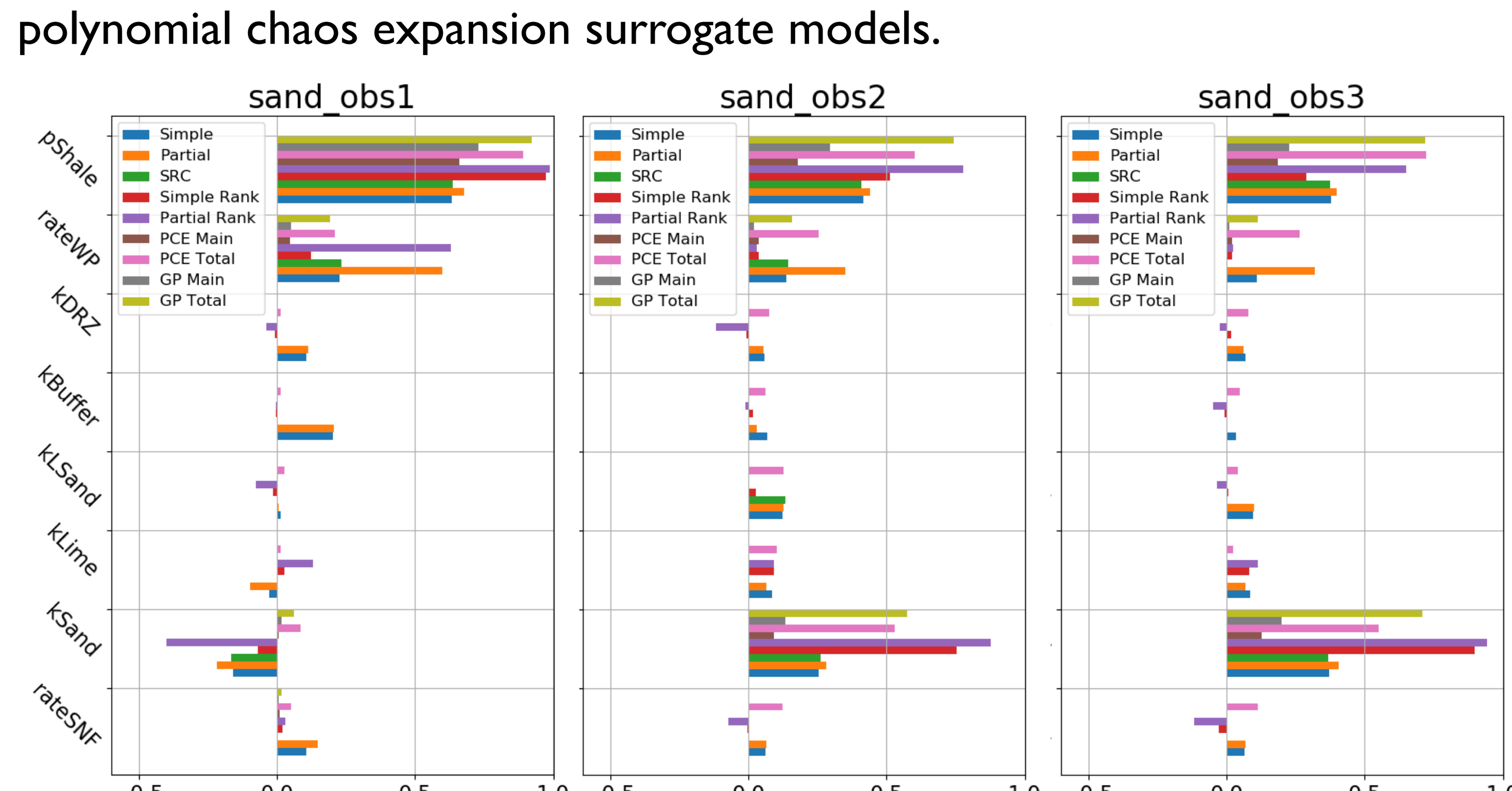

Figure 4. Sensitivity of maximum ^{129}I concentration to sampled inputs.

Implications

All SA methods identify pShale and kSand as the input variables having the greatest effect on the output variable of interest – maximum ^{129}I concentration at downgradient points in the sandstone aquifer (Figure 4). This result suggests that, given the constraints of the simulations performed for the clay reference case PA, reduction of uncertainty in these input variables would most reduce the uncertainty in the output variable. For pShale, kSand, and rateWP, the total sensitivity index is several times larger than the main sensitivity index, indicating the importance of parameter interactions. The finding of near zero total sensitivity indices for kDRZ, kBuffer, kLime, and kLSand indicates that values of these input variables could be fixed without affecting uncertainty in maximum ^{129}I concentration at observation points in the upper sandstone aquifer.

References

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